Since 2006 this series of successful workshops has been held in both Germany and the USA. Its goal is to bring together scientists from various scientific fields to bridge the gap between biological simulations at the molecular level and approaches to describe biological systems at the cellular level and beyond.

This year’s fifth workshop will take place from 20 to 22 July 2011, again at the Research Centre Jülich, jointly organized by the Jülich Supercomputing Centre (JSC), the German Research School for Simulation Sciences (GRS), and Michigan Technological University (MTU). It is dedicated to Harold Scheraga who will celebrate his 90th birthday later this year. Dr. Scheraga pioneered the use of computers in chemistry and biology. His work inspired many of the research areas that are the topic of this meeting.

In the spirit of Harold Scheraga’s work, this workshop will bring together researchers from physics, chemistry, biology, and computer science to acquaint each other with current trends in computational biophysics and systems biology, to explore avenues of cooperation, and to establish together a detailed understanding of cells at a molecular level. Its main focus will be on:

- Protein folding and aggregation,
- Multi-protein complexes and supramolecular assemblies,
- Cellular environments and interaction networks,

and on Models, Algorithms, and High Performance Computing. The workshop will act as a platform for in-depth discussion of cutting-edge research results obtained by international scientists at all levels in their careers. Invited talks will highlight recent algorithmic developments in and successful applications of HPC to life sciences. A limited number of contributed talks and a poster session will allow participants at an early stage of their career to discuss their ongoing research and to put it into the context of the workshop. Finally, several panel sessions will stimulate the exchange of views between the various scientific fields and the different approaches to understanding the biological systems in question.

For the full program see http://www2.fz-juelich.de/conference/cbsb11; there also links to the programs and proceedings of the earlier workshops can be found.

This volume contains 27 contributions to the 4th Russian-German Advanced Research Workshop on Computational Science and HPC presented in October 2009 in Freiburg, Germany. The workshop was organized jointly by the HLRS, the Institute of Computational Technologies of the Siberian Branch of the Russian Academy of Sciences (ICT SB RAS) and the Section of Applied Mathematics of the University of Freiburg (IAM Freiburg). The contributions range from computer science, mathematics and HPC to applications in mechanical and aerospace engineering. They show a wealth of theoretical work and simulation experience with a potential of bringing together theoretical mathematical modelling and usage of high performance computing systems presenting the state of the art of computational technologies.


This volume contains 27 contributions to the 4th Russian-German Advanced Research Workshop on Computational Science and HPC presented in October 2009 in Freiburg, Germany. The workshop was organized jointly by the HLRS, the Institute of Computational Technologies of the Siberian Branch of the Russian Academy of Sciences (ICT SB RAS) and the Section of Applied Mathematics of the University of Freiburg (IAM Freiburg). The contributions range from computer science, mathematics and HPC to applications in mechanical and aerospace engineering. They show a wealth of theoretical work and simulation experience with a potential of bringing together theoretical mathematical modelling and usage of high performance computing systems presenting the state of the art of computational technologies.


Service-oriented Infrastructures including Grid and Cloud Computing are technologies in a critical transition to wider adoption by business. Their use may enable enterprises to achieve optimal IT utilization, including sharing resources and services across enterprises and on-demand utilization of those made available by business partners over the network. This book is an essential reference for researchers and practitioners in service-oriented IT. It analyses a selection of common capabilities (services capturing reusable functionality of IT solutions) that have been applied to tackle challenging business problems and were validated by the BEinGRID consortium in real-life business trials covering most European market sectors.